

Clusterization of deformation modes for quantitative evaluation on factor analysis techniques on statistical shape modelling

Abstract. Statistical shape analysis techniques commonly employed in the medical imaging community rely on Factor Analysis (FA) techniques to decompose shape variability into a reduced set of interpretable components. In this paper we present a quantitative study of the interpretability capabilities of two of these FA techniques, namely Principal Component Analysis (PCA) and Principal Factor Analysis (PFA). The study builds on a clusterization method based on the minimization of an energy term computed on the vector field describing each mode of deformation along a surface. The method was tested on a dataset composed by left human femur Computerized Tomography (CT) 3-D images. Statistics were drawn to measure quantitatively the interpretability of PCA and PFA shape variability decomposition.

1 Introduction

The analysis of shape variability of anatomical structures is of key importance in a number of clinical disciplines, as abnormality in shape can be related to certain diseases. Examples in neurology include the study of brain asymmetry to verify its relation to schizophrenia [1], or the detection and quantification of atrophy as a correlate to multiple sclerosis. These techniques have also proven to be useful to decrease the invasiveness of surgical procedures and increase their accuracy and safety (e.g., [2]).

Statistical shape analysis techniques enjoy a remarkable popularity within the medical image analysis community. Its flagship, the Active Shape Model (ASM), proposed by Cootes et al. [3], provides a method to study the structure of point data sets or meshes [1]. This technique was later extended to intensity information, and thus image data, as the Active Appearance Model (AAM) [4]. Nearly all existing statistical shape analysis methods rely on Principal Component Analysis (PCA) to build a compact model of principal ‘modes of variation’ from a training set. PCA belongs to a family of methods for multivariate analysis commonly known as Factor Analysis (FA). Reviews and comparative studies of FA techniques can be found in [5–7]. Such techniques can be classified into linear and non-linear, reflecting whether the shape variation can be expressed as a linear combination of basic deformation primitives. We contend that a factorial decomposition of shape variability, if it is to be easily interpretable, must follow

a linear model, where each mode of variation has a scalar weight. PCA is a linear technique.

In a previous work we performed a qualitative study between PCA and another linear factor analysis technique known as Principal Factor Analysis (PFA). The study was performed on datasets of different nature (i.e., data dimensionality, image modality, studied anatomical structure, etc.) [8]. On the results obtained, one aspect that prevents full evaluation of these techniques is the lack of methods to quantify interpretability. With current analyses being based in more or less intuitive aspects (e.g., visual inspection of a single image or a sequence of images), the outcome is dependent to the observer. Furthermore, the 3-D characteristic of the data makes difficult a qualitative analysis of results, which is important when one wants to compare results from different FA-based techniques [8]. In this work we present a comparative study between PCA and PFA aiming to measure quantitatively their interpretability capabilities. For this, our main hypothesis is that the degree of interpretability of a certain shape variability decomposition is directly related to the homogeneity of the deformation field across the surface for each mode of deformation. Based on this, this study relies on a technique aimed to cluster a vector field describing a mode of deformation across a surface. The clusterization technique is based on the minimization of an energy composed by two terms: a first term based on the co-linearity among vector directions and a second term that considers the area gain when adding a candidate point to a cluster. Furthermore, the magnitude of deformation at each point is considered as well in order to give more importance to points having larger displacements.

Sections two and three present PCA and PFA respectively, then in section four, the clusterization algorithm of a non-uniform deformation vector field across a surface is described. Section five provides results on real data of human femur Computerized Tomography (CT) images. Finally, section six ends with discussions and conclusions.

2 Principal Component Analysis

PCA is a projection model for FA, aiming at finding a low-dimensional manifold in the space of the data, such that the distance between the data and its projection on the manifold is small [6]. PCA is the best, in the mean-square error sense, linear dimension reduction technique [5]. Given a set of training data t_1, t_2, \dots, t_N in a given orthonormal basis of \mathbb{R}^D , PCA finds a new orthonormal basis u_1, \dots, u_D with its axes ordered. This new basis is rotated such that the first axis is oriented along the direction in which the data has its highest variance. The second axis is oriented along the direction of maximal variance in the data, orthogonal to the first axis. Similarly, subsequent axes are oriented so as to account for as much as possible of the variance in the data, subject to the constraint that they must be orthogonal to the preceding axes. Consequently, these axes have associated decreasing values λ_d , $d = 1, \dots, D$, corresponding to the variance of the data set when projected on the axes. The principal compo-

nents are the set of new ordered basis vectors. The way to compute the principal components is to compute the sample covariance matrix of the data set, S , and then find its eigen-structure $S = U\Lambda$. Where U is a $D \times D$ matrix which has the unit length eigenvectors u_1, \dots, u_D as its columns, and Λ is a diagonal matrix with the corresponding eigenvalues $\lambda_1, \dots, \lambda_D$. The eigenvectors are the principal components and the eigenvalues their corresponding projected variances [6].

3 Principal Factor Analysis

In opposition to PCA, which is a projection model, PFA can be considered as a generative model for FA. Generative models try to model the density function that is assumed to have generated the data, under a set of constraints that restricts the set of possible models to those with a low intrinsic dimensionality [6, 7]. PFA represents an observed D -dimensional continuous variable, t , as a linear function f of an L -dimensional ($L \leq D$) continuous latent variable x and an independent Gaussian noise process:

$$t = Ax + \mu + e \quad (1)$$

Here A is the $D \times L$ factor loading matrix defining the linear function f , μ is a D -dimensional vector representing the mean of the distribution of t , and e is a D -dimensional vector representing the noise or individual variability associated with each of the D observed variables. PFA assumes a Gaussian distributed prior and noise model, and a linear mapping from data space to latent space.

The columns of the $D \times L$ matrix A are referred to as factor loadings.

The data space noise model e is normal centered in $f(x)$ with diagonal covariance matrix Ψ :

$$p(t|x) \sim N(f(x), \Psi) \quad (2)$$

The D diagonal elements of Ψ are referred to as the uniqueness. Following Bayes rule, the posterior in latent space is also normal:

$$p(x|t) \sim N(A(t - \mu), (I + A^t \Psi^{-1} A)^{-1}), \quad (3)$$

with

$$A = A^t (\Lambda A^t + \Psi)^{-1} = (I + A^t \Psi^{-1} A)^{-1} \quad (4)$$

The parameters of the PFA model may be estimated using the EM (Expectation-Maximization) algorithm [9]:

- E-step: This requires computing the moments. For each data point t_n given the current parameter values at iteration τ $A^{(\tau)}$ and $\Psi^{(\tau)}$:

$$E\{x|t_n\} = A^{(\tau)}(t_n - \mu) \quad (5)$$

$$E\{xx^t|t_n\} = I - A^{(\tau)}\Lambda^{(\tau)} + A^{(\tau)}(t_n - \mu)(t_n - \mu)^t(A^{(\tau)})^t \quad (6)$$

- M-step: This results in the following update equations for the factor loadings Λ and uniqueness Ψ :

$$\Lambda = \left(\sum_{n=1}^N t_n E\{x|t_n\}^t \right) \left(\sum_{n=1}^N E\{xx^t|t_n\}^t \right)^{-1} \quad (7)$$

$$\Psi^{(\tau+1)} = \frac{1}{N} \text{diag} \left(\sum_{n=1}^N t_n t_n^t - \Lambda^{(\tau+1)} E\{x|t_n\}^t t_n^t \right) \quad (8)$$

Where the updated moments are used and the ‘diag’ operator sets all off-diagonal elements of a matrix to zero. The location parameter μ is estimated by the sample mean, and does not take part in the EM algorithm.

Note that as opposed to PCA, the factor decomposition is not unique, since an orthogonal rotation of the factors ($\Lambda' = \Lambda R$ where R is an orthogonal matrix) does not alter the distribution in data space, $p(t)$. Thus, from all the factor loading matrices Λ , we are free to choose that which is easiest to interpret according to some criterion. We employ Varimax rotation [10], which finds an orthogonal rotation of the factors and maximizes the sparseness of the retained modes such that, for each new factor, the loadings are either very large or very small (in absolute value). The resulting rotated matrix Λ' has many values clamped to (almost) 0, that is, each factor involves only a few orthogonal variables. This has been found to simplify interpretation [11].

4 Clusterization of a vector field across a surface

The output result from the generation of the statistical models using PCA and PFA is a point distribution model (PDM) able to describe, provided a triangulation of these points, the shape variability of the structure under study as a surface embedded in the 3-D space. Let $P = \{p_1, \dots, p_M\}$, $M \in \mathcal{N}^*$, be the set of points of our PDM, and $T = \{\tau_1, \dots, \tau_N\}$, $N \in \mathcal{N}^*$, the triangulation connecting points in P that generate a mesh surface embedded in a domain $D \in \mathbb{R}^3$. For each point $p_i \in P$, $i = 1, \dots, M$, a vector \mathbf{V}_i can be computed as

$$\mathbf{V}_i = \mathbf{v}_i^+ - \mathbf{v}_i^-, \quad (9)$$

with

$$\mathbf{v}_i^+ = \bar{\mathbf{m}} + \alpha_j \Phi_j \quad (10)$$

$$\mathbf{v}_i^- = \bar{\mathbf{m}} - \alpha_j \Phi_j \quad (11)$$

Right sides in equations (10) and (11) denote the generic PDM model generated from either PCA or PFA, where $\bar{\mathbf{m}}$ corresponds to the mean shape and α_j is a scaling value for the j th principal mode or principal factor of the eigen-matrix or factor loadings matrix Φ_j . The scalar value α_j is chosen accordingly to the plausible range of values that generate valid shapes within the PDM training dataset (e.g. $\pm 3\sqrt{\lambda_j}$ for PCA).

What follows concerning the clusterization across the surface given its triangulation, was initially inspired in the work presented in [12], which was conducted for vector field segmentation of moving objects in 2-D image sequences. Here we extend this work to unstructured 3-D displacement vector field across a surface following some key ideas presented in our previous work [13], where methods were presented to perform clusterization of triangulated surfaces based on some surface properties like normal direction at each triangle, size of triangles, etc.

Let us define the mapping function \mathcal{M} as

$$\begin{aligned} \mathcal{M} : T &\rightarrow \mathbb{R}^{+*} \times S^4 \\ \tau_i &\mapsto (a_i, \mathbf{V}^{(1)}, \mathbf{V}^{(2)}, \mathbf{V}^{(3)}); i = 1, \dots, N \end{aligned} \quad (12)$$

Where a_i is the area covered by triangle τ_i , and $\mathbf{V}^k, k = \{1, 2, 3\}$, vectors at each vertex of triangle τ_i , computed as in eq. (9).

The clusterization process can be seen as a minimization problem where we minimize the following functional over a region or domain $\Omega \subseteq D$:

$$\mathcal{C} = \operatorname{argmin}_{\Omega} J(\mathcal{M}(\Omega)), \quad (13)$$

where $J(\cdot)$ is an energy term composed by two components: a first energy component takes into account the co-linearity between vectors within the domain Ω and the predominant vector direction \mathbf{V}_{Ω} in Ω , weighted by the vector length in order to give more importance to regions having a stronger deformation. The second term acts as a maximal area constraint. The energy $J(\cdot)$ has then the following form:

$$J(\mathcal{M}(\Omega)) = \int_{\Omega} \left(\frac{|\mathbf{V}_{\Omega} \times \mathbf{V}(m)|}{|\mathbf{V}(m)|} \right)^2 \frac{L_{max}}{|\mathbf{V}(m)|} dm + \gamma \int_{D \setminus \Omega} dm, \quad (14)$$

where γ is a real value and $L_{max} = \max_D \{|\mathbf{V}(\mathbf{m})|\}$.

The dominant vector direction \mathbf{V}_{Ω} is found as the highest eigenvalue of the following matrix [12]:

$$M(\Omega) = \int_{\Omega} \mathbf{V}(m) \mathbf{V}^t(m) dm \quad (15)$$

Minimization of (13) is performed by means of a hierarchical scheme, where each pattern is first considered as a cluster and then they are iteratively visited and agglomerated according to the energy measure J until all triangles $\tau_i, i = \{1, \dots, N\}$ in T have been analyzed [13, 14].

5 Results

We present results obtained from a training set of 30 surface models extracted from CT data. These models represent complete left human femurs, and are used in on-going research at our institute for computer-assisted surgery, such as total hip replacement (THR), total knee arthroplasty (TKA), and anterior cruciate ligament surgery (ACL). Correspondences across data sets were established

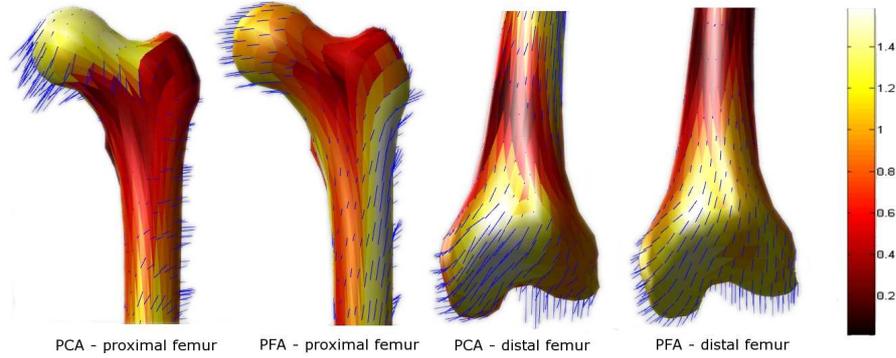


Fig. 1. Shape variability decomposition of left femurs using PCA and PFA. Lines correspond to vector directions describing the second mode of deformation, whereas the magnitude of deformation has been mapped as colors on the surface. Only proximal and distal sections of femur are shown in order to enhance visualization.

with a spherical harmonic (SPHARM) based shape representation method [15]. These correspondences are further optimized via a Minimum Description Length (MDL) optimization [16].

For both, PCA and PFA, the first mode describes the change in length of femurs. More interesting are the second to fourth modes. Figure 1 shows the second mode using PCA and PFA. From Fig. 1 it can be shown that PFA yields a more homogeneous deformation than PCA. While this can be easily seen in the femoral head and around the condyles in the distal femur, a qualitative evaluation on the whole femur is not an easy task due to the local variations, vector magnitudes, and the fact of visualizing 3-D information in a 2-D space. This turns to be more difficult for the third and fourth modes, where deformations are more subtle and complex, requiring more experience from the observer.

The clusterization algorithm was applied to the shape variability decompositions using PCA and PFA. The obtained clustered triangulated surfaces are colored for their differentiation. Fig. 5 shows the results obtained for mode number two. It can be seen that the clusterization on the PFA shape variability decomposition has larger clusters than for PCA, indicating the increased homogeneity of the shape decomposition of PFA over PCA. Figure 5 plots for both, PCA and PFA, the number of clusters produced at different levels of γ (Eq. (14)), which regulates the desired degree of homogeneity of each cluster. As expected, at different values of γ the number of clusters required by PFA is smaller than for PCA, indicating the higher homogeneity of the deformation pattern obtained with PFA. This same behavior occurs as well for mode three and four.

In another experiment, for each mode of decomposition, the parameter γ (Eq. (14)) was adjusted in order to generate the same number of clusters for PCA and PFA. Ten sets were generated ranging from 20 to 40 clusters. Then, the mean standard deviation of vector directions across clusters was computed. The results indicate that for the second mode of PCA and PFA, the mean standard

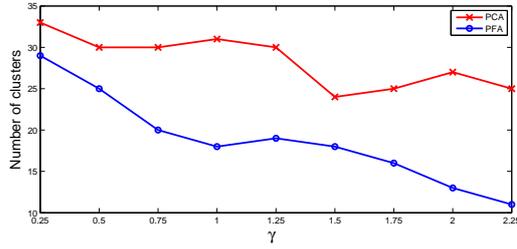


Fig. 2. Number of clusters obtained for PCA and PFA with different values of parameter γ (Eq. (14)). It can be seen that at different ‘degrees of homogeneity’ the number of clusters required by PFA to describe the deformations is always smaller than for PCA.

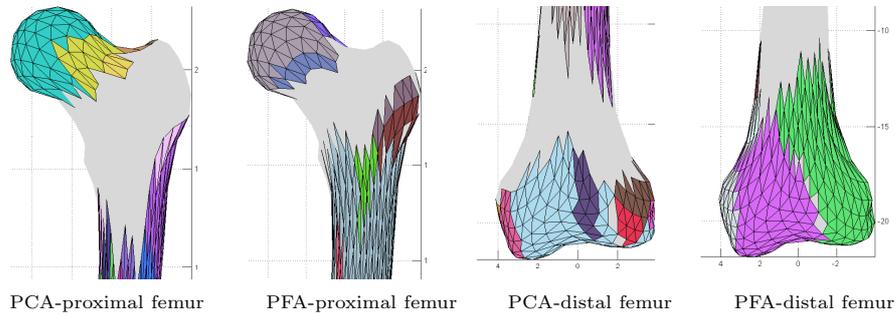


Fig. 3. Clusterization results for second mode of PCA and PFA. On each figure, each cluster has a particular color (chosen randomly). Gray regions correspond to triangle cells having low deformations and so not considered as part of a cluster (see red regions in Fig. 1).

deviation was 0.40 and 0.24, respectively. Similarly, for third mode of PCA and PFA, the standard deviation was 0.43 and 0.36, respectively, and of 0.52 and 0.32 for mode number four. These figures show once again the increased homogeneity across clusters for PFA over PCA.

6 Conclusions

A clusterization technique aimed to quantitatively study the interpretability characteristics of PCA and PFA was presented. We contend that a shape variability decomposition is easier to interpret when the shape deformation presents more regular or homogeneous patterns across the surface. The results on femur data allowed us to conclude in quantitative terms that PFA decomposition is easier to interpret, results that agree with the qualitative results obtained in a previous study [8]. We do not claim that PFA should replace PCA, but it should be considered as a complementary tool when studying shape variability. Clinical applications of the proposed technique include, for instance, its utilization on bone implant design. In this scenario, being able to characterize a shape defor-

mation in terms of its preferred direction and the region of interest where this deformation is predominant could greatly improve the implant design process.

References

1. González-Ballester, M.A., Zisserman, A., Brady, M.: Measurement of brain structures based on statistical and geometrical 3D segmentation. In: *Proc. of MICCAI 1998, Lecture Notes in Computer Science*. Volume 1496. (1998) 499–508
2. Rajamanim, K.T., Styner, M., Talib, H., Zheng, G., Nolte, L., Styner, M., González-Ballester, M.A.: Statistical deformable bone models for robust 3D surface extrapolation from sparse data. *Medical Image Analysis* **11**(2) (2007) 99–109
3. Cootes, T.F., Taylor, C.J., Cooper, D.H., Graham, J.: Active shapemodells - their training and applications. In: *Computer Vision and Image Understanding*. Volume 61. (1995) 38–59
4. Cootes, T.F., Edwards, G.J., Taylor, C.J.: Active appearance models. *IEEE Transactions on Pattern Analysis and Machine Intelligence* **23**(6) (2001) 681–685
5. Fodor, I.: A survey of dimension reduction techniques. Lawrence Livermore National Laboratory Technical Report no. UCRL-ID-148494 (2002)
6. Svensén, J.F.M.: GTM: The Generative Topographic Mapping. Phd thesis, Aston University (1998)
7. Carreira-Perpiñan, M.A., Renals, S.: Dimensionality reduction of electropalatographic data using latent variable models. *Speech Communication* **26**(4) (1998)
8. (Anonymous)
9. Rubin, D.B., Thayer, D.T.: EM algorithms for ML factor analysis. *Psychometrika* **47**(1) (1982) 69–76
10. Kaiser, H.F.: The varimax criterion for analytic rotation in factor analysis. *Psychometrika* **23**(3) (1958) 187–200
11. Darryl, C., Colin, F.: Kernel factor analysis with varimax rotation. (In: *Neural Networks, 2000. IJCNN 2000*) 381–386
12. Roy, T., Barlaud, M., Debreuve, E., Aubert, G.: Vector field segmentation using active contours: Regions of vectors with the same direction. In: *Workshop on Variational, Geometric, and Level Set Methods in Computer Vision (VLSM)*. (200)
13. (Anonymous)
14. Jain, A.K., Murty, M.N., Flynn, P.J.: Data clustering: a review. *ACM Comput Surv* **31**(3) (1999) 264–323
15. Brechbühler, C., Gerig, G., Kübler, O.: Parametrization of closed surfaces for 3-d shape description. *Computer Vision and Image Understanding* **61** (1995) 154–170
16. Davies, R.H., Twining, C.J., Cootes, T., Waterton, J.C., Taylor, C.J.: A Minimum Description Length approach to statistical shape modelling. *IEEE Transactions on Medical Imaging* **21**(5) (2002) 525–537